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Complex formation in Cu(II)-thioamide-carbonyl compound systems in ethanol solutions

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Abstract

The structures of metal complexes formed in systems Cu(II)-thioamide- carbonyl compounds in water-ethanol solutions were studied by spectroscopic and quantum-chemical methods. It was found that in systems containing thiocarbohydrazide, the processes of template synthesis in water-ethanol solution and in gelatin-immobilized matrices differ substantially. In the case of dithiooxamide and dithiomalonamide, no products of template synthesis were detected; these amides give with the Cu2+ ion the chelate complexes with a ratio Cu2+: ligand = 1: 2 and with the N2S 2 coordination core for dithiooxamide and S4 coordination core for dithiomalonamide. The quantum-chemical calculations in terms of the density functional theory were shown to adequately describe the structures of metal complexes and relative thermodynamic characteristics of the template synthesis processes in the systems under study. © Pleiades Publishing, Inc., 2006.

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